KN08 | DIFFUSE SCATTERING - PAST, PRESENT AND FUTURE.

Welberry, Richard (Australian National University, Canberra, AUS)

Whereas analysis of Bragg peaks provides information about the average crystal structure (atomic coordinates, site-occupancies, or mean-square atomic displacements — *single* site properties), diffuse scattering contains information about how *pairs* of atoms behave and is thus potentially rich source of information on how atoms and molecules interact. Crystallographers have been aware of diffuse scattering since the earliest times, but development of techniques for recording and analysing it have lagged well behind the advances made in conventional crystallography.

A major impediment to the utilisation of this rich source of information is the diversity and often complex combination of disorder effects that arise in nature and the fact that until recently no one simple method of analysis has been available which can usefully deal with all of them. In this talk we show how computer simulation of a model crystal *does* provide such a general method by which diffuse scattering of all kinds and from all types of materials can be interpreted and analysed. Such methods have only been feasible since the advent of powerful and relatively inexpensive computers.

To trace these developments examples of different real materials are discussed. For organic systems the goal has been to move toward a truly quantitative solution where a pixel-by-pixel comparison between observed and calculated intensities gives agreement factors comparable to those achieved for Bragg intensities. For inorganic systems such as the ferroelectrics PZN and PMN there has been a move towards constructing atomistic potentials that allow diffuse scattering to be calculated *a priori*.